Lattice investigation of inhomogeneous phases in the Gross-Neveu model

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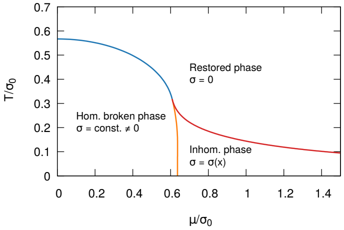
Introduction (1)

- **Long-term goal** (for many researchers in our field): Compute the phase diagram of QCD.
  - Extremely difficult ...
  - ... e.g. "sign problem" in lattice QCD for chemical potential $\mu \neq 0$, computations very challenging/impossible.
- **QCD-inspired models in the $N_f \to \infty$ limit**:

  QCD-inspired = symmetries similar as in QCD, e.g. chiral symmetry
  $N_f \to \infty$ limit = infinite number of flavors
  - Inhomogeneous phases at large μ and small temperature T.

    inhomogeneous phase = phase with a spatially non-constant order parameter
  - Analytical results for the Gross-Neveu (GN) model in 1+1 dimensions.

    [O. Schnetz, M. Thies and K. Urlichs, Annals Phys. **314**, 425 (2004) [hep-th/0402014]]
- **Are there inhomogeneous phases in QCD?**



Introduction (2)

- Project "**Inhomogeneous phases at high density**" of the CRC-TR 211 "**Strong-interaction matter under extreme conditions**" (universities of Bielefeld, Darmstadt, Frankfurt):
  - Goals:
    - Study the phase diagrams of various QCD-inspired models (GN, chiral GN, Nambu-Jona-Lasinio (NJL), quark-meson model) with particular focus on inhomogeneous phases.
    - Are there inhomogeneous phases in 2+1 or 3+1 dimensions?
    - Are there inhomogeneous phases with 2- or 3-dimensional modulations?
    - Determine the spatial modulation of the condensates (= order parameters) without using specific ansätze (e.g. no restriction to a chiral density wave).
    - Phase structure not only with respect to μ and T but also isospin and strangeness chemical potential μ_I, μ_S.
    - Are there inhomogeneous phases at finite N_f?
  - Methods:
    - Lattice field theory.
      * Lattice field theory computations in the $N_f \rightarrow \infty$ limit (this talk).
      * Lattice field theory simulations at finite N_f (this talk).
    - Functional Renormalization Group (not part of this talk ... M. Buballa, D. Rischke, ...).

Outline

1. Part 1: 2+1 dimensions, $N_f \to \infty$
   - GN model in 2+1 dimensions
   - Technical aspects
     - Discrete symmetry $\sigma \to -\sigma$ and fermion representation
     - Fermion discretization
     - Efficient computation of $\det(Q)$ and minimization of S_{eff}/N
     - Inhomogeneous phases and finite volume
   - Numerical results

2. Part 2: 1+1 dimensions, finite N_f
   - GN model in 1+1 dimensions
   - Ensembles
   - Numerical results

Part 1:
2+1 dimensions, $N_f \to \infty$

GN model in 2+1 dimensions, $N_f \to \infty$ (1)

- At the moment we study the GN model 2+1 dimensions.
  - Do inhomogeneous phases exist in 2+1 dimensions?
  - Is the phase diagram in 2+1 dimensions similar to the analytically known phase diagram in 1+1 dimensions?
  - Are there inhomogeneous phases with 2-dimensional modulations?

  [M. Winstel, J. Stoll, M. Wagner, arXiv:1909.00064]

- Action:

$$S = \int d^3x \left(\sum_{j=1}^{N_f} \bar{\psi}_j \Big(\gamma_\nu \partial_\nu + \gamma_0 \mu \Big) \psi_j - \frac{g^2}{2} \left(\sum_{j=1}^{N_f} \bar{\psi}_j \psi_j \right)^2 \right).$$

- After introducing a scalar field σ and performing the integration over fermionic fields

$$S_{\text{eff}} = N_f \left(\frac{1}{2\lambda} \int d^3x\, \sigma^2 - \ln \Big(\det(\underbrace{\gamma_\nu \partial_\nu + \gamma_0 \mu + \sigma}_{=Q}) \Big) \right)$$

$$Z = \int D\sigma\, e^{-S_{\text{eff}}},$$

  where $\lambda = N_f g^2$.

- One can show $\sigma \propto \langle \sum_{j=1}^{N_f} \bar{\psi}_j \psi_j \rangle$.

GN model in 2+1 dimensions, $N_f \to \infty$ (2)

- $N_f \to \infty$:
  - Only "a single field configuration" important in $\int D\sigma\, e^{-S_\text{eff}}$ (global minimum of S_eff/N).
  - Assume t-independence of this field configuration, i.e. $\sigma = \sigma(x, y)$.
- For numerical treatment the degrees of freedom have to be reduced to a finite number.

  $\to$ Finite volume and discretization needed.
  - For example lattice field theory.
  - There are other possibilities to discretize, e.g. finite mode discretization, discretization by piecewise polynomial functions, etc.

    [M. Wagner, Phys. Rev. D **76**, 076002 (2007) [arXiv:0704.3023]]
    [A. Heinz, F. Giacosa, M. Wagner, D. H. Rischke, Phys. Rev. D **93**, 014007 (2016) [arXiv:1508.06057]]
- Technical aspects:
  - Discrete symmetry $\sigma \to -\sigma$ and fermion representation: 2-component irreducible versus 4-component reducible representation?
  - Fermion discretization: Fermion doubling problem? Explicit breaking of chiral symmetry? Unphysical zero modes?
  - Efficient computation of $\det(Q)$ and minimization of S_eff/N: After discretization, Q is a large matrix.
  - Inhomogeneous phases and finite volume: Not just exponentially small corrections (size of the inhomogeneous structures versus size of the volume).

Discrete symmetry $\sigma \to -\sigma$ and fermion representation

- One can show $S_{\text{eff}}[+\sigma] = S_{\text{eff}}[-\sigma]$ (i.e. S_{eff} has a discrete symmetry).
- $\sigma \propto \langle \sum_{j=1}^{N_f} \bar{\psi}_j \psi_j \rangle$.
- **1+1 dimensions**:
  - A possible irreducible 2×2 representation for the γ matrices is

$$\gamma_0 = \sigma_1 \quad , \quad \gamma_1 = \sigma_2 .$$

  - $\sigma \neq 0$ would indicate spontaneous breaking of the symmetry $\psi_j \to \sigma_3 \psi_j$.
  - Since σ_3 anticommutes with γ_0 and γ_1, it is appropriate to define $\gamma_5 = \sigma_3$ and to interpret the symmetry as discrete chiral symmetry.
- **2+1 dimensions**:
  - A possible irreducible 2×2 representation for the γ matrices is

$$\gamma_0 = \sigma_1 \quad , \quad \gamma_1 = \sigma_2 \quad , \quad \gamma_2 = \sigma_3 .$$

  - It is impossible to find a corresponding appropriate γ_5 matrix, i.e. a matrix, which anticommutes with γ_0, γ_1 and γ_2.
  - Consequently, a non-vanishing σ cannot be interpreted as a signal for chiral symmetry breaking.
  - A possibility to retain the interpretation of σ as chiral order parameter is to use a reducible 4×4 representation.
  - One can show that the phase diagrams for the irreducible 2×2 representation and the reducible 4×4 representation are identical.

Fermion discretization (1)

- Various discretizations tested.
- Expansion in a set of basis functions, e.g. plane waves,

$$\psi(x,t) \quad \rightarrow \quad \sum_{m_t,m_x} c_{m_t,m_x} e^{i(p_{m_t} t + p_{m_x} x)} \quad , \quad \sigma(x) \quad \rightarrow \quad \sum_{m_x} d_{m_x} e^{i p_{m_x} x}$$

with $p_{m_t} = 2\pi(m_t - 1/2)/L_t$, $p_{m_x} = 2\pi m_x/L_x$, $d_{m_x} = (d_{-m_x})^*$.

[M. Wagner, Phys. Rev. D **76**, 076002 (2007) [arXiv:0704.3023]]

$(-)$ Requires $\det(Q) = \det(Q^\dagger)$, not the case e.g. for $\mu_I \neq 0$ or $\mu_s \neq 0$.

- $\det(Q) \rightarrow \det(\langle f_n | Q | f_{n'} \rangle)$, where f_n are basis functions, e.g. $f_{m_t,m_x} = e^{i(p_{m_t} t + p_{m_x} x)}$.
- Problem: $\mathrm{span}\{f_n\} \neq \mathrm{span}\{Q f_n\}$, which causes artificially small eigenvalues or zero modes in $\langle f_n | Q | f_{n'} \rangle$ not present in Q.
  $\rightarrow$ Wrong and weird results.
- Increasing the number of basis functions does not cure the problem.
- Solution: $\ln(\det(Q)) \rightarrow (1/2)\ln(\det(Q^\dagger Q))$ (requires $\det(Q) = \det(Q^\dagger)$).

$(-)$ Number of spatial modes in $\psi(x,t)$ should be larger than number of modes in $\sigma(x)$.

- Q depends on $\sigma(x)$; basis functions representing $\psi(x,t)$ must be able to resolve more detail for an accurate approximation of $\det(Q)$.

$(+)$ No fermion doubling.

$(+)$ Resulting condensates $\sigma(x)$ are continuous functions.
(When using lattice field theory, $\sigma(x)$ is represented by a set of points σ_x.)

Fermion discretization (2)

- Lattice discretization:
  - Naively discretized fermions.

$$\psi(x,t) \quad \rightarrow \quad \psi_{x,t} \quad , \quad \partial_x \psi(x,t) \quad \rightarrow \quad \frac{\psi_{x+a,t} - \psi_{x-a,t}}{2a} \quad , \quad \ldots$$

    $(x, t = 0, a, 2a, \ldots;$ a: lattice spacing).

    $(-)$ Fermion doubling.
  - Naively discretized with non-symmetric derivatives.

    $(-)$ No fermion doubling, but other severe problems.
  - Staggered fermions.

    [P. de Forcrand and U. Wenger, PoS LATTICE **2006**, 152 (2006) [hep-lat/0610117]]

    $(-)$ Fermion doubling still present.
  - ...
- Most promising seems to be a combination of two approaches:
  - Plane wave expansion in t direction.

    $(+)$ Easy analytical simplifications possible, e.g. $\det(Q)$ factorizes.
  - Naive lattice discretization in x direction.

    $(+)$ Fermion doubling not a problem in the large-N limit ("$2 \times \infty = \infty$").

$$\psi(x,t) \quad \rightarrow \quad \psi_x(t) \quad = \quad \sum_m \psi_{x,m} e^{ip_m t} \quad , \quad \sigma(x) \quad \rightarrow \quad \sigma_x .$$

Efficient computation of $\det(Q)$ and ...

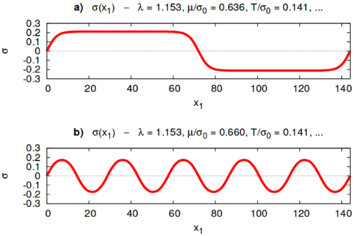
- $Q = \gamma_\nu \partial_\nu + \gamma_0 \mu + \sigma$ is a large matrix, e.g. $\mathcal{O}(10^5) \times \mathcal{O}(10^5)$ entries.
- Efficient computation of $\det(Q)$ and minimization of

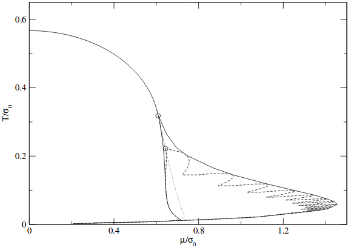
$$\frac{S_{\text{eff}}}{N_f} = \left(\frac{1}{2\lambda} \int d^2x\, \sigma^2 - \ln\Big(\det(Q)\Big)\right)$$

  need
  - preparatory analytical simplifications, e.g. to factorize $\det(Q)$,
  - efficient algorithms and codes.
- Work in progress.
- Details are rather technical, beyond the scope of this presentation.

Inhomogeneous phases and finite volume (1)

- Periodic modulation of the inhomogeneous condensate, wave length λ depends on (μ, T) (left figure [for 1+1 dimensions]).
- Extent of the finite volume L typically fixed.
- If L is a multiple of λ, i.e. $L \approx n\lambda$, $n \in \mathbb{N}_+$
  no particular problems with the finite volume, correct results.
- If $L \approx (n - 1/2)\lambda$, $n \in \mathbb{N}_+$
  modulation of the inhomogeneous condensate does not fit into the finite volume, severely distorted results (see right figure, oscillating dashed line).





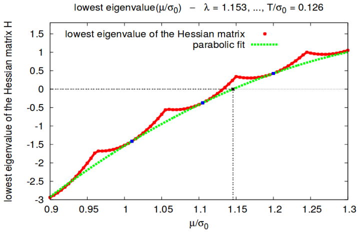
right figure [for 1+1 dimensions] from [P. de Forcrand and U. Wenger, PoS LATTICE **2006**, 152 (2006) [hep-lat/0610117]]

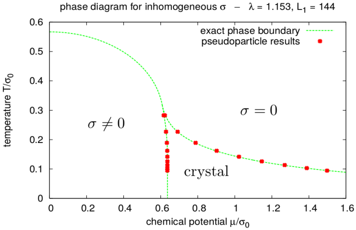
Inhomogeneous phases and finite volume (2)

- Infinite volume phase boundaries can be extracted from finite volume results.
- Phase boundary between inhomogeneous phase and restored phase:
  - Characterized by the appearance/disappearance of negative eigenvalues of the Hessian matrix

$$H_{xy} = \frac{\partial}{\partial \sigma_x} \frac{\partial}{\partial \sigma_y} S_{\text{eff}} \bigg|_{\sigma=0} .$$

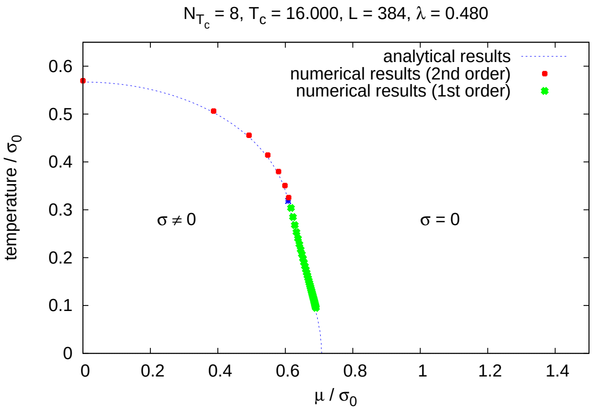
  - Lowest eigenvalue of H as a function of μ oscillates in a finite volume (red curve in left figure):
    - Minima: $L \approx n\lambda$, $n \in \mathbb{N}_+$, essentially identical to the infinite volume result.
    - Maxima: $L \approx (n - 1/2)\lambda$, $n \in \mathbb{N}_+$, significantly different from the infinite volume result.
  - Fitting a smooth curve (e.g. a 2nd order polynomial) from below (green curve in left figure [for 1+1 dimensions]) approximates the infinite volume result.





Numerical results, 1+1-dimensional GN model (1)

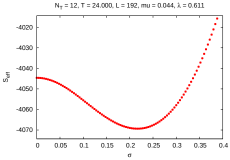
- Phase diagram with restriction to homogeneous condensate σ.
  (A Test of our method and implementation.)

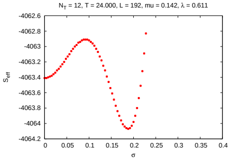


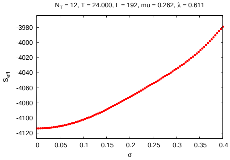
analytical results first obtained in [U. Wolff, Phys. Lett. B **157**, 303 (1985)]

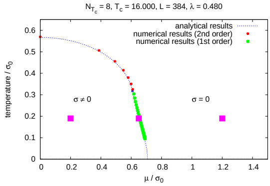
Numerical results, 1+1-dimensional GN model (2)

- $S_{\text{eff}}(\sigma)$ for homogeneous condensate σ.
  - Left: far inside the broken phase ($\mu/\sigma_0 = 0.20$, $T = T_c/3$).
  - Center: in the broken phase close to the 1st order phase boundary ($\mu/\sigma_0 = 0.65$, $T = T_c/3$).
  - Right: in the symmetric phase ($\mu/\sigma_0 = 1.20$, $T = T_c/3$).



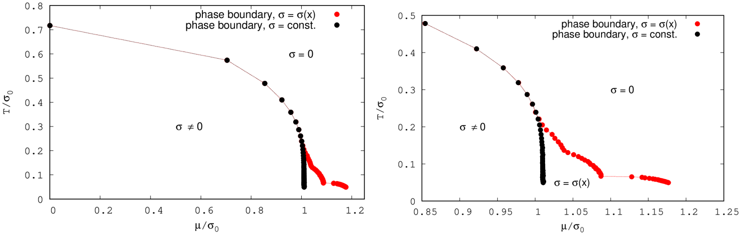






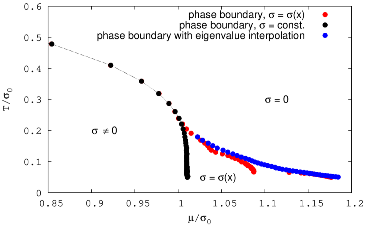
Numerical results, 2+1-dimensional GN model (1)

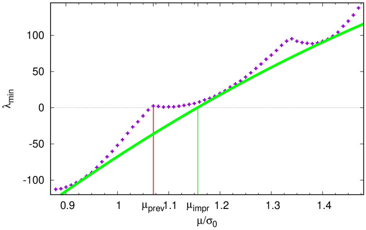
- Phase diagram:
  - **Black dots**: restriction to homogeneous condensate $\sigma = \mathrm{const}$ (in agreement with available analytical results).
    [K. Urlichs, PhD thsis, University of Erlangen-Nuremberg (2007)]
  - **Red dots**: restriction to 1-dimensional modulations, $\sigma = \sigma(x)$.
    - Phase boundary via eigenvalues of the Hessian matrix ("stability analysis").
    - At finite volume, i.e. no extrapolation to infinite volume.



Numerical results, 2+1-dimensional GN model (2)

- Phase diagram:
  - **Black dots**: restriction to homogeneous condensate $\sigma = \mathrm{const}$.
  - **Red dots**: restriction to 1-dimensional modulations, $\sigma = \sigma(x)$.
    - Phase boundary via eigenvalues of the Hessian matrix ("stability analysis").
    - At finite volume, i.e. no extrapolation to infinite volume.
  - **Blue dots**: restriction to 1-dimensional modulations, $\sigma = \sigma(x)$.
    - Phase boundary via eigenvalues of the Hessian matrix ("stability analysis").
    - Extrapolated to infinite volume (see right figure; smallest eigenvalue of the Hessian matrix as a function of μ at fixed T).

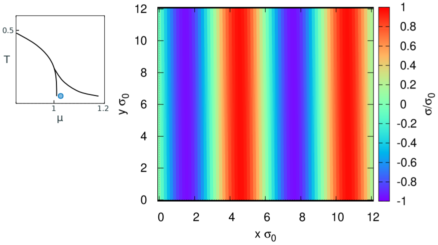


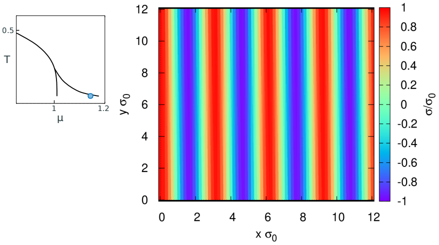


Numerical results, 2+1-dimensional GN model (3)

- Directions of instability for the condensate in the inhomogeneous phase at
  - $(\mu/\sigma_0, T/\sigma_0) = (1.025, 0.055)$ (left figure)
  - $(\mu/\sigma_0, T/\sigma_0) = (1.166, 0.055)$ (right figure)

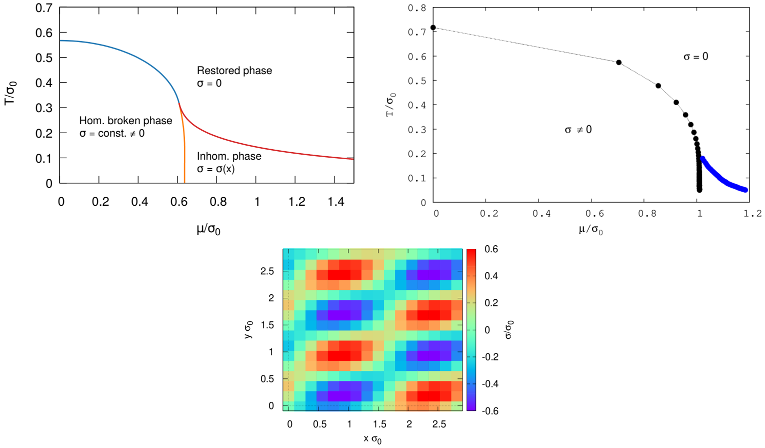
  (restriction to 1-dimensional modulations, $\sigma = \sigma(x)$).
- For increasing μ the wavelength decreases (as for the 1+1-dimensional GN model).





Numerical results, 2+1-dimensional GN model (4)

- Comparison of the phase diagram of the 1+1-dimensional (left figure) and the 2+1-dimensional (right figure) GN model.
  - Inhomogeneous phase in 2+1 dimensions smaller than for 1+1 dimensions.
  - Could become larger, when allowing 2-dimensional modulations, $\sigma = \sigma(x, y)$ ...?



Next steps

- Explore lattice spacing dependence in detail.
  (Results were obtained at a single lattice spacing. Recent results from a Ginzburg-Landau stability analysis with a Pauli-Villars regularization as well as crude lattice results indicate a strong cutoff dependence ... the inhomogeneous phase might even disappear in the continuum limit.)
- Are there inhomogeneous phases with 2-dimensional modulations?
- Extend studies to 3+1 dimensions.
- Study the phase diagram of more realistic QCD-inspired models (chiral GN, Nambu-Jona-Lasinio (NJL), quark-meson model, ...) with particular focus on inhomogeneous phases.
  $\rightarrow$ Phase structure not only with respect to μ and T but also isospin and strangeness chemical potential μ_I, μ_S ...?

Part 2: 1+1 dimensions, finite N_f

GN model in 1+1 dimensions, finite N_f (1)

- At the moment we study the GN model 1+1 dimensions.
  - Do inhomogeneous phases exist in 1+1 dimensions at finite N_f?
  - Is the phase diagram similar to the analytically known phase diagram for $N_f \to \infty$?

[L. Pannullo, J. Lenz, M. Wagner, B. Wellegehausen and A. Wipf, arXiv:1902.11066]
[L. Pannullo, J. Lenz, M. Wagner, B. Wellegehausen and A. Wipf, arXiv:1909.11513]

- Action:

$$S = \int d^2x \left(\sum_{j=1}^{N_f} \bar{\psi}_j \Big(\gamma_\nu \partial_\nu + \gamma_0 \mu \Big) \psi_j - \frac{g^2}{2} \left(\sum_{j=1}^{N_f} \bar{\psi}_j \psi_j \right)^2 \right).$$

- After introducing a scalar field σ (= condensate) and performing the integration over fermionic fields

$$S_{\text{eff}} = N_f \left(\frac{1}{2\lambda} \int d^2x\, \sigma^2 - \ln \Big(\det(\underbrace{\gamma_\nu \partial_\nu + \gamma_0 \mu + \sigma}_{=Q}) \Big) \right)$$

$$Z = \int D\sigma\, e^{-S_{\text{eff}}},$$

where $\lambda = N_f g^2$.

- One can show $\langle \sigma \rangle \propto \langle \sum_{j=1}^{N_f} \bar{\psi}_j \psi_j \rangle$, i.e. $\langle \sigma \rangle$ is proportional to the chiral condensate.

GN model in 1+1 dimensions, finite N_f (2)

- Simulations with two different fermion discretizations, which do not break chiral symmetry:
  - **Naive fermions**:

$$\partial_\mu^{\rm naive}(x,y) \quad = \quad \frac{\delta_{x+e_\mu,y} - \delta_{x-e_\mu,y}}{2a}.$$

    - N_f is a multiple of 8 (because of HMC algorithm and fermion doubling).
  - **SLAC fermions**:

$$\partial_\mu^{\rm SLAC}(x,y) \quad = \quad \Big(1 - \delta_{x,y}\Big) \frac{\pi}{N_\mu} \frac{(-1)^{x_\mu - y_\mu}}{\sin((x_\mu - y_\mu)\pi/N_\mu)}$$

$$\rightarrow \quad \mathcal{F}\Big(\partial_\mu^{\rm SLAC}\psi\Big)(p) \quad = \quad i p_\mu \mathcal{F}\Big(\psi\Big)(p).$$

    - N_f is a multiple of 2 (because of HMC algorithm; no fermion doubling).
    - Non-local, rarely used, ...

      [S. D. Drell, M. Weinstein and S. Yankielowicz, Phys. Rev. D **14**, 487 (1976)]

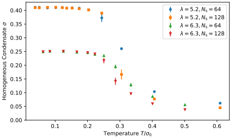
$\rightarrow$ Important cross-check of numerical results (for $N_f = 8$).
$\rightarrow$ Allows to study also a small number of fermion flavors, $N_f = 2$.

Ensembles

- Simulation of a large number of ensembles:

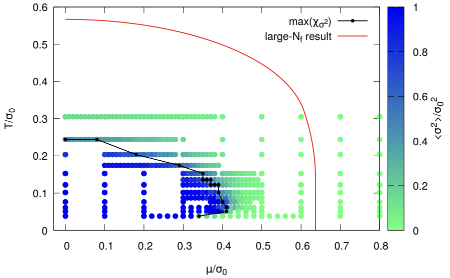
N_f	$N_t = 1/Ta$	$N_s = L/a$	λ_{naive}	$a\sigma_0$	λ_{SLAC}	$a\sigma_0$
2	$4, 6, \ldots, 24, 28, 32, 40, \ldots, 64$	64	—	—	1.022	0.4100(5)
8	$4, 6, \ldots, 24, 28, 32, 40, \ldots, 64, 80$	32, 64, 128	3.91	0.4096(3)	5.20	0.4100(5)
			4.84	0.2527(3)	6.20	0.2495(5)
			5.28	0.2015(3)	6.85	0.195(5)
16	$4, 6, \ldots, 24, 28, 32, 40, \ldots, 64$	64	—	—	10.7	0.4100(5)

- Scale setting via
$$\sigma_0 = \lim_{L \to \infty} \left\langle |\overline{\sigma}| \right\rangle \Big|_{\mu=0,\, T=0} \qquad \left(\overline{\sigma} = \frac{1}{N_t N_s} \sum_{t,x} \sigma(x,t) \right).$$
("the condensate at $\mu = 0$ and $T = 0$ deep inside the homogeneously broken phase").



$\langle\overline{\sigma}^2\rangle$, homogeneously broken phase ($N_f = 8$)

- $\langle\overline{\sigma}^2\rangle$ can distinguish a homogeneously broken phase from a symmetric phase and an inhomogeneous phase.
- Homogeneously broken phase at $N_f = 8$ (blue region) has similar shape as for $N_f \to \infty$ (indicated by the red line), but is smaller (plot for naive fermions).



Correlation function $C(x)$ ($N_f = 8$) (1)

- $\langle \sigma(t,x) \rangle$ might not be suited to detect an inhomogeneous phase ("inhomogeneous field configurations" could be spatially shifted relative to each other).
- Use spatial correlation function

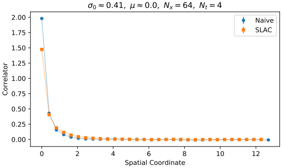
$$C(x) = \frac{1}{N_t N_s} \sum_{t,y} \Big\langle \sigma(t, y+x) \sigma(t,y) \Big\rangle,$$

to detect a possibly existing inhomogeneous phase.

- Expectation:
  - Symmetric phase: $C(x) \sim 0$.
  - Homogeneously broken phase: $C(x) \sim \sigma_0^2$.
  - Inhomogeneous phase: $C(x)$ is an oscillating function (similar to a kink-antikink or a cosinus).

Correlation function $C(x)$ $(N_f = 8)$ (2)

symmetric phase (large T)
$(\mu/\sigma_0, T/\sigma_0) \approx (0.0, 0.610)$

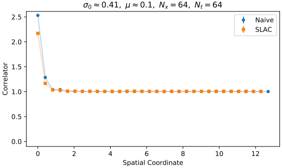


- Spatial correlation function

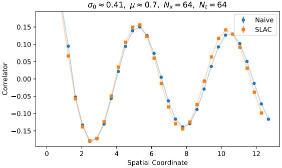
$$C(x) = \frac{1}{N_t N_s} \sum_{t,y} \Big\langle \sigma(t, y + x)\sigma(t, y) \Big\rangle .$$

- Wavelength in the inhomogeneous phase decreases for increasing μ (as for $N_f \to \infty$).
- Agreement of naive and SLAC fermions.

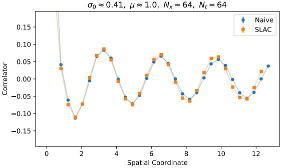
hom. broken phase (small T, small μ)
$(\mu/\sigma_0, T/\sigma_0) \approx (0.1, 0.038)$



inhomogeneous phase (small T, large μ)
$(\mu/\sigma_0, T/\sigma_0) \approx (0.7, 0.038)$

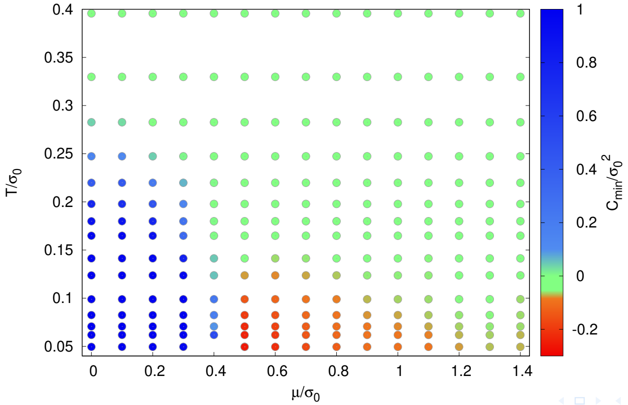


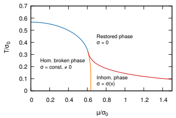
inhomogeneous phase (small T, large μ)
$(\mu/\sigma_0, T/\sigma_0) \approx (1.0, 0.038)$



Correlation function $C(x)$, phase diagram ($N_f = 8$)

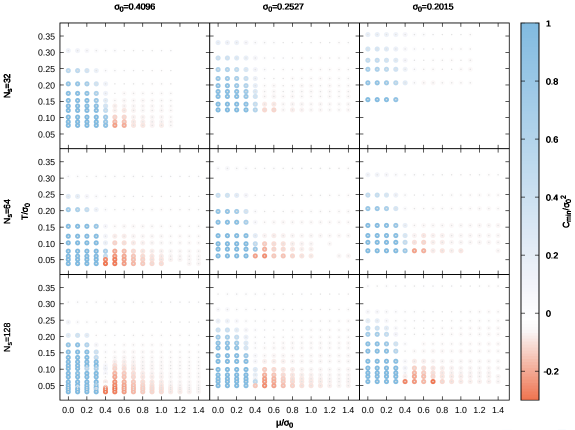
- Phase diagram via
$$\min_x C(x) \begin{cases} \approx 0 & \text{inside a symmetric phase} \\ \gg 0 & \text{inside a homogeneously broken phase} \\ \ll 0 & \text{inside an inhomogeneous phase} \end{cases}$$
(plot for naive fermions).
- Similar to the $N_f \to \infty$ phase diagram.





"Continuum and infinite volume limit" ($N_f = 8$)

- Increasing spatial volume (at fixed lattice spacing): top to bottom. $\downarrow$
- Decreasing lattice spacing (at constant spatial volume): top left to bottom right. $\searrow$
- Phase diagram stable under variations of the lattice spacing and the spatial volume (plots for naive fermions).

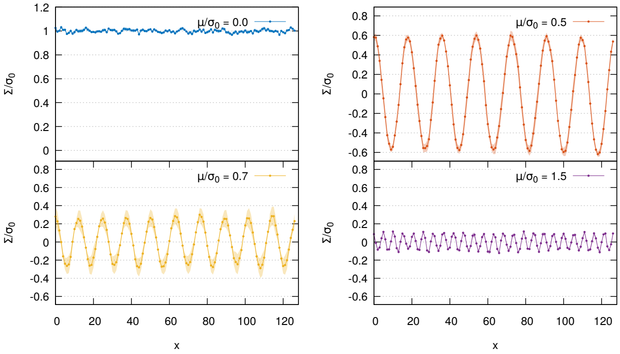


Aligned condensate $\Sigma(x)$ ($N_f = 8$)

- Aligned condensate: field configurations are matched by spatial translations $x \to x - \Delta x$, before the ensemble average is computed,

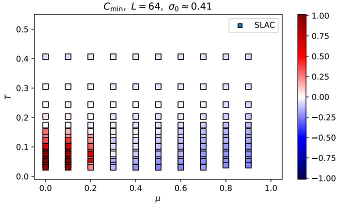
$$\Sigma(x) = \frac{1}{N_t} \sum_{t=0}^{N_t} \Big\langle \sigma(t, x - \Delta x) \Big\rangle.$$

- Suited to visualize both homogeneous and inhomogeneous condensates (plots for SLAC fermions, $T/\sigma_0 = 0.031$).



N_f dependence

- Phase diagram for $N_f = 2$ (SLAC fermions).



- $\langle|\overline{\sigma}|\rangle$ at $\mu = 0$ for $N_f \in \{2, 8, 16\}$ and for $N_f \to \infty$.